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Infrared synchrotron study of high pressure-temperature chemical reaction products from supercritical methanol

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Beamline(s): U2A

Introduction: Our high-pressure experimental team at LLNL has recently discovered how to initiate pure supercritical fluid reactions at hundreds of degrees Celsius and at pressures of GPa [1].

Results and Discussion: In one example supercritical methanol (T = 250 °C) is subjected to 532nm and 1064 nm 100 ps pulses at 5 GPa. When the temperature is increased at a constant 5 GPa a reaction proceeds to form supercritical water, carbon dioxide, ethane, and perhaps methane. These products were discerned using beamline U2A synchrotron FTIR line (Fig. 1). Water and carbon-rich products separate and form bubbles (Fig. 2). The control study we ran where methanol was not laser-treated yielded only water and carbon dioxide products and no bubbles. In both studies we took samples up to 400°C and 5 GPa. (Carbon-13 pressure sensor was used above 250 °C). These same products are predicted by the CHEETAH thermo-chemical code if no carbon, in the form of diamond, is produced. The results of our future experiments at different P-T conditions will be particularly valuable in validating the kinetics capability of the CHEETAH thermo-chemical code.

References: 1. J. M. Zaug *et al*. Unpublished.

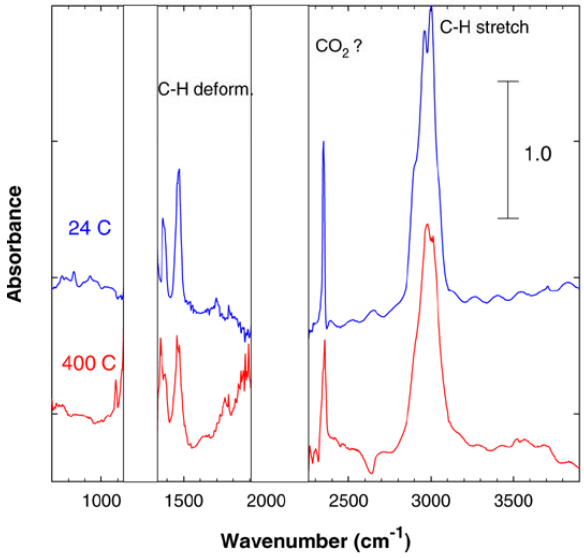

Figure 1. FTIR spectrum of MeOH in the ethane-rich product region of the DAC showing the formation of both ethane and CO_2.

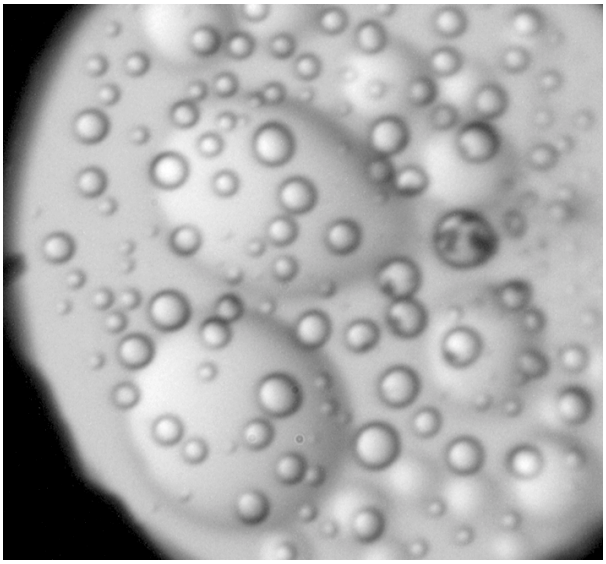

Figure 2. Photomicrograph of supercritical methanol, reacted at 598K showing immiscible fluid phase